$Zn_{22}Zr$ Structure: A22B_cF184_227_cdfg_a-001

This structure originally had the label `A22B_cF184_227_cdfg_a`. Calls to that address will be redirected here.

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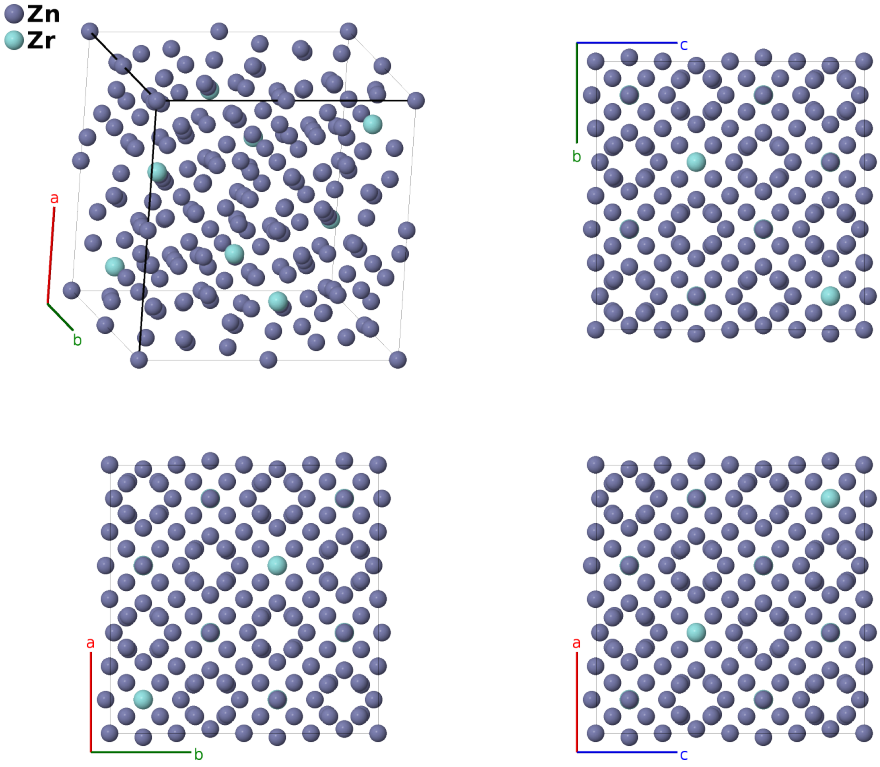
https://aflow.org/p/MX6R

https://aflow.org/p/A22B_cF184_227_cdfg_a-001



Prototype	$Zn_{22}Zr$
AFLOW prototype label	A22B_cF184_227_cdfg_a-001
ICSD	106238
Pearson symbol	cF184
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A22B_cF184_227_cdfg_a-001 --params=`a, x_4, x_5, z_5

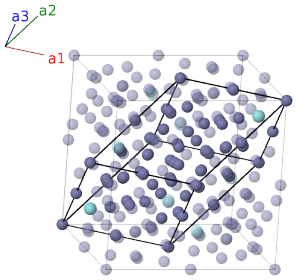
Other compounds with this structure

$Be_{22}Mo$, $Be_{22}Re$, $Be_{22}W$, $Al_{18}Cr_2Mg_3$, $Ce(TiAl_{10})_2$, $Dy(RhZn_{10})_2$, $U(VAl_{10})_2$, $Y(RuZn_{10})_2$

- (Samson, 1961) gives the atomic coordinates in terms of setting 1 of space group $F\bar{4}dm$ #227. We have shifted this to the standard setting 2, where the inversion site of the lattice is at the origin.
- Samson also suggests that the "$Zn_{14}Zr$" structure is created when zirconium atoms replace some of the zinc atoms on the (16c) site [the (16d) site in Samson's orientation].
- This structure can be derived from the $Mg_3Cr_2Al_{18}$ structure.

Face-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Zr I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	Zr I
$\mathbf{B_3}$	=	0	=	0	(16c)	Zn I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Zn I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Zn I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Zn I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Zn II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(16d)	Zn II
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Zn II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16d)	Zn II
$\mathbf{B_{11}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{16}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{17}}$	=	$\left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_4 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{19}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{20}}$	=	$\left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{21}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(48f)	Zn III

$\mathbf{B_{22}}$	=	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+a\left(x_4+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Zn III
$\mathbf{B_{23}}$	=	$z_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2+(2x_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{24}}$	=	$z_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{25}}$	=	$(2x_5-z_5)\,\mathbf{a}_1-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{26}}$	=	$-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1+(2x_5-z_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{27}}$	=	$(2x_5-z_5)\,\mathbf{a}_1+z_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{28}}$	=	$-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{29}}$	=	$z_5\,\mathbf{a}_1+(2x_5-z_5)\,\mathbf{a}_2-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{30}}$	=	$z_5\,\mathbf{a}_1-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+(2x_5-z_5)\,\mathbf{a}_3$	=	$-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{31}}$	=	$z_5\,\mathbf{a}_1+(2x_5-z_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{32}}$	=	$z_5\,\mathbf{a}_1-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{33}}$	=	$-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2+(2x_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{34}}$	=	$(2x_5-z_5)\,\mathbf{a}_1+z_5\,\mathbf{a}_2-\left(2x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{35}}$	=	$-z_5\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{36}}$	=	$-z_5\,\mathbf{a}_1-z_5\,\mathbf{a}_2-(2x_5-z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{37}}$	=	$-(2x_5-z_5)\,\mathbf{a}_1+\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{38}}$	=	$\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1-(2x_5-z_5)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{39}}$	=	$-(2x_5-z_5)\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{40}}$	=	$\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2-(2x_5-z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{41}}$	=	$-z_5\,\mathbf{a}_1-(2x_5-z_5)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{42}}$	=	$-z_5\,\mathbf{a}_1+\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{43}}$	=	$-z_5\,\mathbf{a}_1-(2x_5-z_5)\,\mathbf{a}_2+\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{44}}$	=	$-z_5\,\mathbf{a}_1+\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-(2x_5-z_5)\,\mathbf{a}_3$	=	$a\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{45}}$	=	$\left(2x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Zn IV
$\mathbf{B_{46}}$	=	$-(2x_5-z_5)\,\mathbf{a}_1-z_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(96g)	Zn IV

References

[1] S. Samson, *The Crystal Structure of the Intermetallic Compound $ZrZn_{22}$*, Acta Cryst. **14** (1961), doi:10.1107/S0365110X61003600.

Found in

[1] T. B. Massalski, H. Okamoto, P. R. Subramanian, and L. Kacprzak, eds., *Binary Alloy Phase Diagrams*, vol. 3 (ASM International, Materials Park, Ohio, USA, 1990), 2^{nd} edn. Hf-Re to Zn-Zr.